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## Disclaimer

# Overbarrier model with electron back-capture

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We present an extension of the classical overbarrier model [F. Sattin, Phys. Rev. A **62**, 042711 (2000)] to include the effect of electron back-capture. Back-capture is the process by which an electron that has already been captured by the projectile ion is re-captured by the target atom. Back-capture reduces the overall electron capture cross section, especially at low velocity. When the binding energy of the projectile is less than that of the target, the cross section falls substantially at low velocity, which is in accord with experimental data.

Keywords:

## I. INTRODUCTION

The classical overbarrier model is a simple analytic model that describes the charge exchange between a target atom or ion and a projectile ion [1–6]. In the literature, the model and all of its variations predict that the electron capture cross section is a monotonically decreasing function of velocity [5–10]. In fact, the analytic formula shows that the model predicts close to a $1/v$ velocity dependence when ionization is neglected. With ionization, the falloff with velocity is stronger.

Experiments, however, reveal that the cross section as a function of velocity can contain a local maximum (see for instance [11, 12] or Figs. 1 and 2 of this paper, which reproduce some of the data in [11, 12]). We contend that the model fails to correctly predict the velocity dependence below this maximum because it neglects back-capture, the process in which a target electron is captured by the projectile but then captured back by the target all within the same collision. A comprehensive model should take into account the possibility of capture proceeded by back-capture, proceeded by capture again, etc., all within the same collision.

In general, a target atom with a large binding energy holds its electron tightly so that the probability for electron capture by a projectile is low. In the context of the overbarrier model, the back-capture process is similar to the capture process, but with the roles of the projectile and target reversed. Thus, the probability for back-capture must be inversely proportional to the binding energy of the projectile ion. At low collison velocity, then, where there is enough time for many capture and back-capture processes, the electron should preferentially end up bound to the object (the target or projectile) with the greatest binding energy. So, when the binding energy of the projectile is much lower than that of the target, it is reasonable to expect a large decrease in the electron capture cross section at low velocity. This is generally true in experiment [11, 12], and we show it is also true in the overbarrier model with back-capture included.

## II. REVIEW OF THE OVERBARRIER MODEL

The overbarrier model has several versions which vary in the details. We use the version that can be found in [5, 6, 13]. These references provide particularly nice derivations of the model. To review, consider an electron bound in the potential well of a target where the core of the target has effective charge $Z_t$. As a projectile ion with charge $Z_p$ approaches to an internuclear distance $R$, its potential well overlaps with that of the target creating a saddle-shaped potential field. In the plane of the three particles, we use the cylindrical coordinate system of [6] in which the internuclear axis is labelled with coordinate $z$ and the electron's distance from this axis is labelled with coordinate $\rho$. Then, the total (kinetic plus potential) energy of the electron (in atomic units) is

$$E = \frac{p^2}{2} - \frac{Z_t}{\sqrt{\rho^2 + z^2}} - \frac{Z_p}{\sqrt{\rho^2 + (R-z)^2}}. \qquad (1)$$

When the electron is bound to the target, and in the limit $R \to \infty$, the energy of the electron is approximated as

$$E(R) = -E_t - \frac{Z_p}{R} \qquad (2)$$

where $E_t$ is the binding energy of the target electron in the absence of the projectile.
The saddle-shaped potential is a maximum along the internuclear axis at the distance

$$z_0 = \frac{\sqrt{Z_t}}{\sqrt{Z_t} + \sqrt{Z_p}} R \qquad (3)$$

The electron is able to reach the saddle point if its maximum excursion is equal to $z_0$. This occurs when the internuclear spacing $R$ is less than some maximum

$$R_m = \frac{\alpha\sqrt{Z_p Z_t} + Z_t}{E_t}. \qquad (4)$$

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This expression is derived from Eq. 1 with $z = z_0$ and $\rho = 0$. When $E$ in Eq. 1 is set to $E(R)$ in Eq. 2, $\alpha = 2$; however, if $E = -E_t$, $\alpha = 1$. Sattin showed that $\alpha = 1$ gave better agreement with certain experiments [6, 8]. However, $\alpha = 2$ is consistent with the rest of the model, which always uses the fully perturbed binding energy ($E(R)$ in Eq. 2), so we use $\alpha = 2$ in all calculations.

When $R < R_m$, the electron can cross over the potential barrier at time $t$ and be captured by the projectile if its orbit intersects the potential opening and if the electron is in the part of the orbit that crosses the barrier. The fraction of electron orbits that intersect the opening at time $t$ is given by

$$N_\Omega = \frac{\sqrt{Z_p}}{2\sqrt{Z_t}(\sqrt{Z_t}+\sqrt{Z_p})^2}\left[(\sqrt{Z_t}+\sqrt{Z_p})^2 - Z_p - E_t R\right]. \tag{5}$$

The fraction of electrons that cross any surface perpendicular to their motion within the time interval $dt$ is $dt/T$, where $T$ is the period of the electron orbit:

$$\begin{aligned} T &= 2\int_0^{r_{turn}} \frac{dr}{p} = \sqrt{2}\int_0^{r_{turn}} \frac{dr}{\sqrt{\frac{Z_t}{r} + \frac{Z_p}{|\mathbf{R}-\mathbf{r}|} - E_t - \frac{Z_p}{R}}} \\ &\approx \sqrt{2}\int_0^{1/E_t} \frac{dr}{\sqrt{\frac{Z_t}{r} - E_t}} = \frac{\pi}{\sqrt{2}} Z_t E_t^{-3/2} \end{aligned} \tag{6}$$

where $r = \sqrt{\rho^2 + z^2}$ is the distance of the electron from the target and $r_{turn}$ is the maximum radial excursion of the electron, which occurs when $p = 0$. Note that $p$ is obtained from equating Eqs. 1 and 2. The approximation on the second line of Eq. 6 is then obtained by applying the large $R$ limit (to zeroeth order in $r^2/R^2$), which is consistent with Eq. 2. This is also equivalent to using the momentum without considering the perturbation as was done in [6]. We note that in [8], Sattin mistakenly left out the $Z_p/|\mathbf{R}-\mathbf{r}|$ term in the momentum [14].

As in [6], we use the expression in Eq. 6, but apply a constant corrective factor $1/f_T$ with $f_T \geq 1$ to the period. A justification for this is that we neglect the angular momentum of the electron, but the affect of finite angular momentum is to decrease the period [6]. Otherwise, this is a corrective factor that is needed to make the model results more consistent with experiment.

Next, let $W(t)$ represent the probability for the electron to still be bound to the target at time $t$. Its time rate of change is then given by

$$\frac{dW(t)}{dt} = -N_\Omega \frac{f_T}{T} W(t). \tag{7}$$

Then, the probability for the electron to leak from the target and be captured by the projectile is

$$P_l(b) = 1 - W(\infty) = 1 - \exp\left(-\frac{f_T}{T}\int_{-t_m}^{t_m} N_\Omega \; dt\right). \tag{8}$$

Assuming a straight line collision trajectory with impact parameter $b$ and velocity $v$,

$$R = \sqrt{b^2 + (vt)^2}, \tag{9}$$

the limits of the integral ($\pm t_m$) are derived with $R = R_m$, meaning $-t_m < t < t_m$ is the time range in which charge exchange can occur. The integral in Eq. 8 can be performed analytically due to this known dependence of $R$ on time, meaning the leakage probability can be calculated analytically. The total cross section

$$\sigma = 2\pi \int b P_l(b) db \tag{10}$$

involves an integral which is not normally analytically tractable, so numerical integration is required.

One final consideration of the model is that of ionization. During the collision process, it is possible that the electron is ionized and not captured by the projectile. There are different models within the overbarrier model that have been used to account for ionization [6, 15]. We follow Sattin's, which calculates the electron's binding energy to the projectile while in the saddle point of the potential [6]. This binding energy to the projectile is

$$E_p' = E_t + \frac{Z_p - Z_t}{R} - \frac{v^2}{2} + \frac{v_{et} v^2 t}{R}, \tag{11}$$

$$\text{where} \quad \frac{v_{et}^2}{2} = \frac{(\sqrt{Z_t}+\sqrt{Z_p})^2 - Z_p}{R} - E_t. \tag{12}$$

Note that the binding energy $E_p'$ is not generally equal to the projectile's ground state binding energy $E_p$. The condition for ionization is that $E_p'(t) < 0$, which one can see from Eq. 11 primarily occurs for large $v$ and small or negative $t$. If $E_p'(t) > 0$ for the time interval $t_i < t < t_f$ which is within $\pm t_m$, the capture probability is

$$P_c(b) = 1 - \exp\left(-\frac{f_T}{T}\int_{-t_i}^{t_f} N_\Omega \; dt\right). \tag{13}$$

## III. EXTENSION TO INCLUDE BACK-CAPTURE

Accounting for the return of the electron to the target once it has been captured by the projectile is relatively straight-forward in the case when the projectile is the same element as the target and $Z_p = Z_t$ [16]. It is trickier when the capture and back-capture are not identical processes. To do this calculation, we first define three time-dependent probabilities, $w_t, w_p$, and $w_i$, which represent the probability for the electron to be bound to the target, bound to the projectile, and ionized, respectively. They are constrained in that $w_t + w_p + w_i = 1$.

We can then write evolution equations for each of these probabilities,

$$\begin{aligned}\frac{dw_t}{dt} &= -j_{tp}w_t - j_{ti}w_t + j_{pt}w_p \\ \frac{dw_p}{dt} &= -j_{pt}w_p - j_{pi}w_p + j_{tp}w_t \\ \frac{dw_i}{dt} &= j_{ti}w_t + j_{pi}w_p\end{aligned} \tag{14}$$

where $j_{tp}$ and $j_{pt}$ are the rates of charge exchange from the target to the projectile and from the projectile to the target, respectively, while $j_{ti}$ and $j_{pi}$ are the rates of ionization for an electron bound to the target and to the projectile. Given the initial conditions $w_t = 1, w_p = w_i = 0$ at $t \to -\infty$, the summation constraint ($w_t + w_p + w_i = 1$) is automatically satisfied. The charge exchange and ionization rates are

$$\begin{aligned}j_{tp} &= \frac{f_T}{T_t} N_{\Omega,t}\ \Theta(E'_p)\ \Theta(t_{m,t} - |t|) \\ j_{ti} &= \frac{f_T}{T_t} N_{\Omega,t}\ \Theta(-E'_p)\ \Theta(t_{m,t} - |t|) \\ j_{pt} &= \frac{f_T}{T_p} N_{\Omega,p}\ \Theta(E'_t)\ \Theta(t_{m,p} - |t|) \\ j_{pi} &= \frac{f_T}{T_p} N_{\Omega,p}\ \Theta(-E'_t)\ \Theta(t_{m,p} - |t|)\end{aligned}$$

where $\Theta$ is the Heaviside step function. $T_t, N_{\Omega,t}$, and $t_{m,t}$ are equivalent to $T, N_\Omega$, and $t_m$ from the previous section. The added subscript $t$ simply denotes that they apply to the electron while it is bound to the target. The new variables $T_p, N_{\Omega,p}$, and $t_{m,p}$, denote quantities for the electron bound to the projectile, while $E'_t$ is the counterpart of $E'_p$ – it is the binding energy to the target while in the saddle point, and is not generally equal to $E_t$. To get the expressions for these new variables, simply take all of the expressions in the previous section and exchange the subscripts, $t \to p, p \to t$.

The differential equations (Eqs. 14) must be solved numerically. One point to keep in mind is that the time limits during which the equations must be solved are $-t_{m,t} < t < \max(t_{m,t}, t_{m,p})$. The back-capture may proceed even after the original capture shuts off, or it may shut off before the original capture does. This depends on the relative values of $Z_t, Z_p, E_t$, and $E_p$.

## IV. RESULTS

As a first test case, we look at the electron capture cross section between $N^+$+Ne. Expreimental data from Lo [11] shows that the capture cross section contains a peak at relatively low velocity ($\sim 10^8$ cm/s) as is characteristic when the projectile has lower binding energy than the target ($E_{\rm bind} = 14.5$ eV for N and $E_{\rm bind} = 21.6$ eV for Ne). The experimentally measured cross section as a function of velocity is shown in Fig. 1 along with calculations from the overbarrier model (OBM), in which we set the free parameter $f_T = 5$.

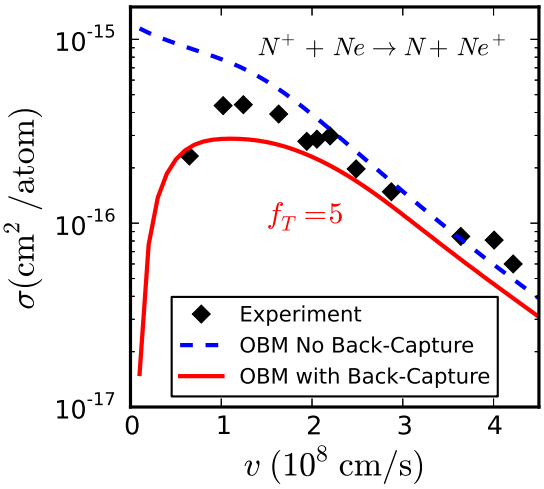


FIG. 1: Comparison of cross section calculations with and without back capture to experimental data [11] for the charge exchange between $N$ and $Ne$. Ionization is included.

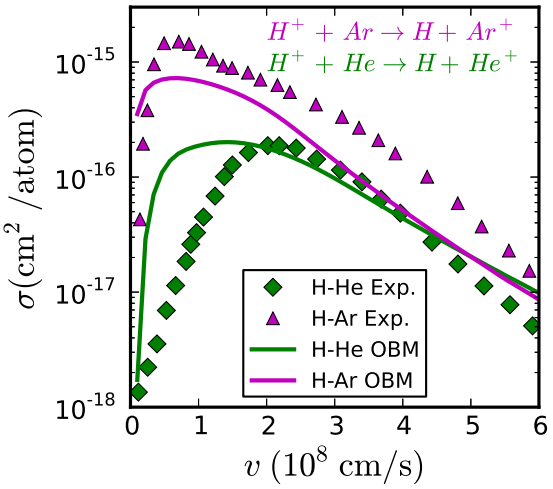


FIG. 2: Comparison of cross section calculations from the overbarrier model with back capture and ionization to experimental data [12].

When back-capture is not included, the overbarrier model is a monotonically decreasing function. With back-capture, there is a peak, allowing for better agreement with experiment at low velocity. The primary effects of increasing $f_T$ are to move the peak in the cross section to higher velocity and to decrease the total cross section. Without applying any rigorous metric, we have chosen $f_T = 5$ because it provides relatively good overall

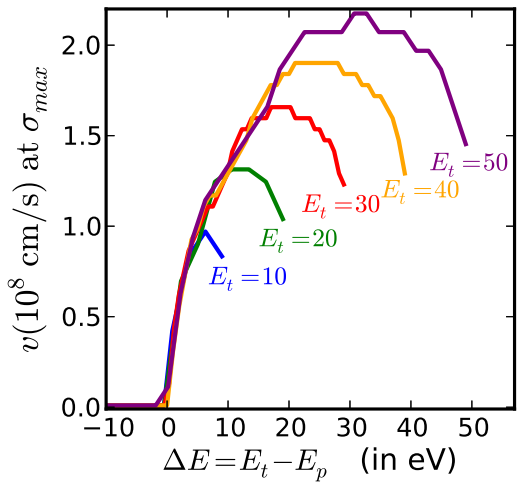


FIG. 3: The velocity at which the cross section curve peaks for the overbarrier model as a function of $\Delta E = E_t - E_p$.

agreement with the experiment.

As a second test case, we compare the full overbarrier model charge exchange cross section calculations to experiments [12] with $H^+$+He and $H^+$+Ar as seen in Fig. 2. Note that $E_{\rm bind} = 13.6$ eV for H, $E_{\rm bind} = 24.6$ eV for He, and $E_{\rm bind} = 15.8$ eV for Ar. Again, we use $f_T = 5$, which gives relatively good, but not necessarily the best agreement between the model and the experiments.

Despite the mediocre agreement, the extended overbarrier model developed here appears to display a property that is consistent with experiment (at least with most of the data in [11, 12]). That is, the velocity at which the cross section peaks is proportional to $\Delta E = E_t - E_p$ as evident in Fig. 2. We show this more clearly for our overbarrier model in Fig. 3, where we plot the velocity at the cross section peak as a function of $\Delta E$. When $\Delta E \leq 0$, there is no peak in the cross section curves (the curves are monotonically decreasing), but for $\Delta E > 0$ the peak velocity grows until $E_p \ll E_t$. Up until $E_p \ll E_t$, there is no dependence on $E_t$, meaning that the particular target and projectile species do not matter. Only the absolute difference in their binding energies matters.

Thus, the overbarrier model with back-capture produces peaked cross section curves when the binding energy of the projectile ion is less than that of the target atom, which is a fairly consistent feature seen in experimental cross section curves. The peak in the cross section curve scales correctly with $\Delta E$; however, the location of the peak does not agree perfectly with experimental data. Overall, the overbarrier model with back-capture provides an improvement over the model without back-capture by taking into account the binding energy of the projectile, albeit at the expense of computational resources.

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